

Usability and Functionality of the Orbitrap Exploris 30K GC-HRMS

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Introduction

The Orbitrap Exploris 30K is MRIGlobal's newest high-resolution GC/MS instrument. As illustrated in Figure 1, the Orbitrap contains a unique type of ion trap mass analyzer that utilizes the precise orbital frequency of ion fragments. It works by trapping ion fragments between two bookend electrodes and forcing them into orbit around a central perpendicular electrode.¹ **The innovative instrument combines the quantitative advantage of triple quadrupole technology with high-resolution scanning abilities. The Orbitrap has full scan, selected ion mode (SIM), and MS/MS capabilities at 30,000 resolution. Other features include a vacuum interlock that allows for source exchange and cleaning while under vacuum, as well as vent-free column exchange.**

TraceFinder functionalities include:

- Processing methods for unknown or target screenings
- Quantitative analyses using in-house compound databases or high-resolution libraries
- Metabolomics profiling
- Impurity testing and identification
- Environmental contaminant scanning and confirmation

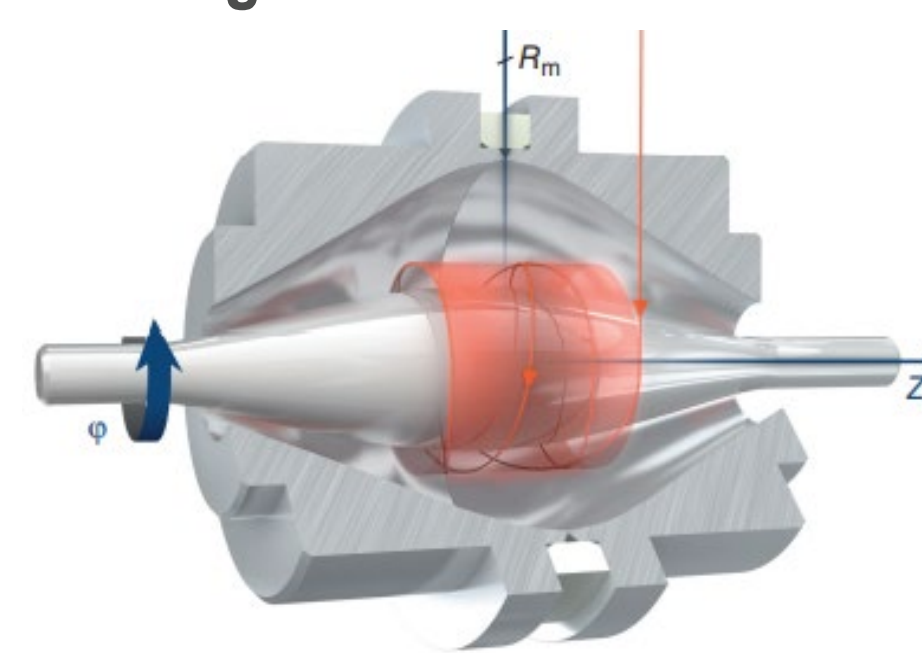


Figure 1. Schematic of the Orbitrap mass analyzer

Hecht, E. S., Etkin, S., Scigelova, M., and Makarov, A., "Fundamentals and advances of orbitrap mass spectrometry," *Encyclopedia of Analytical Chemistry* (September 16, 2019), <https://doi.org/10.1002/9780470027318.a9309.pub2> (accessed March 22, 2022).

Specifications

- Dynamic Range – Quantitative >10E⁶ ; In-spectrum >5,000:1
- Mass Range – 30 to 3000 m/z
- Mass Accuracy – Internal calibration <1 ppm
 - Error(ppm) = Error(Da) x (1,000,000 / m/z of compound)
- Resolution – 30,000
- Scan Rates – Up to 40 Hz at 7,500 resolution at m/z 200
- Sensitivity – Parts-per-trillion concentration

Experiment types:

- MS/MS
- Full Scan
- Selected Ion Monitoring (SIM)

Figure 3. Schematic of Mass Spectrometer on the Orbitrap

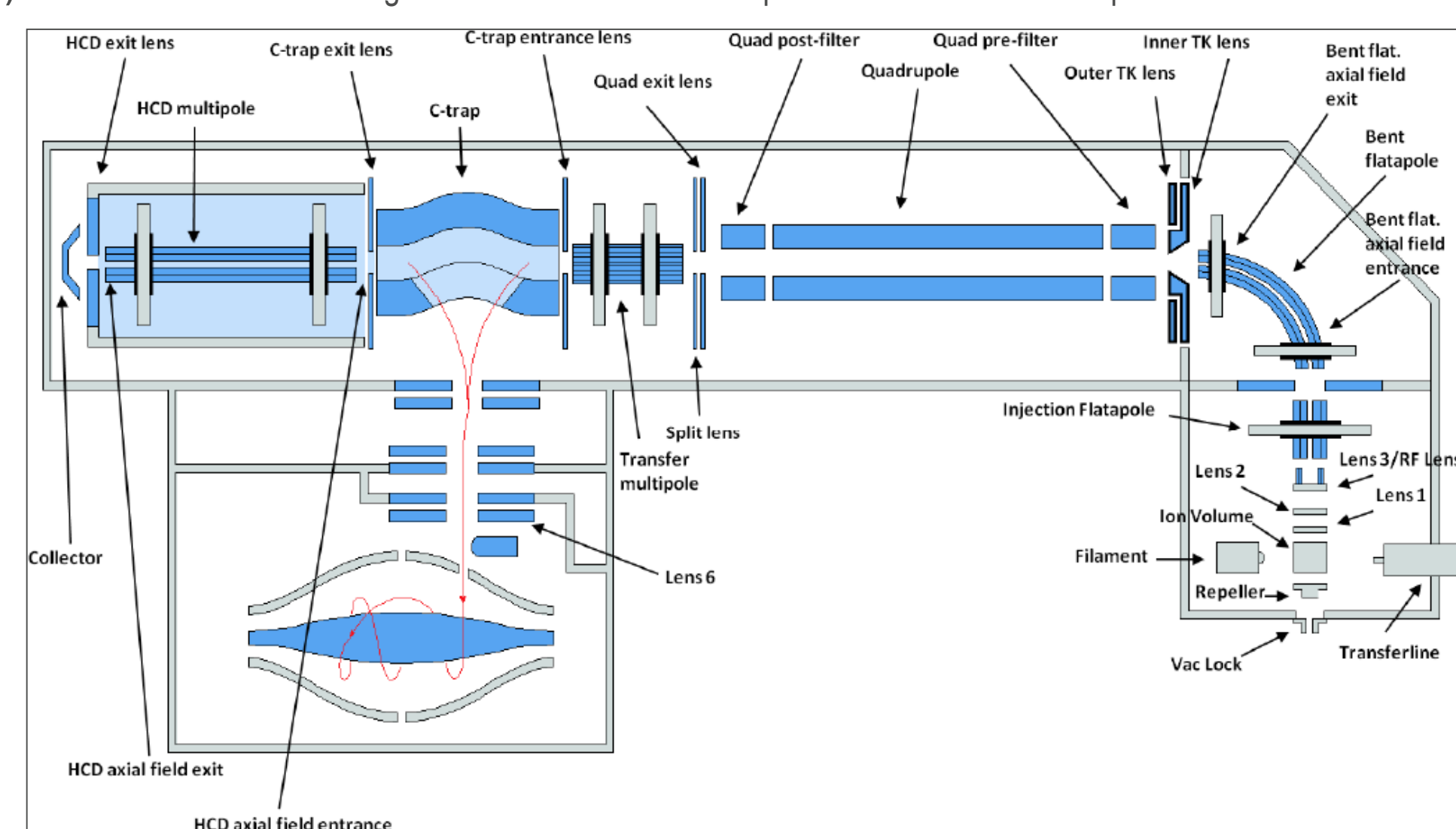


Figure 2. GC-HRMS Orbitrap located in 107S



Initial Evaluation at Thermo Fisher Scientific

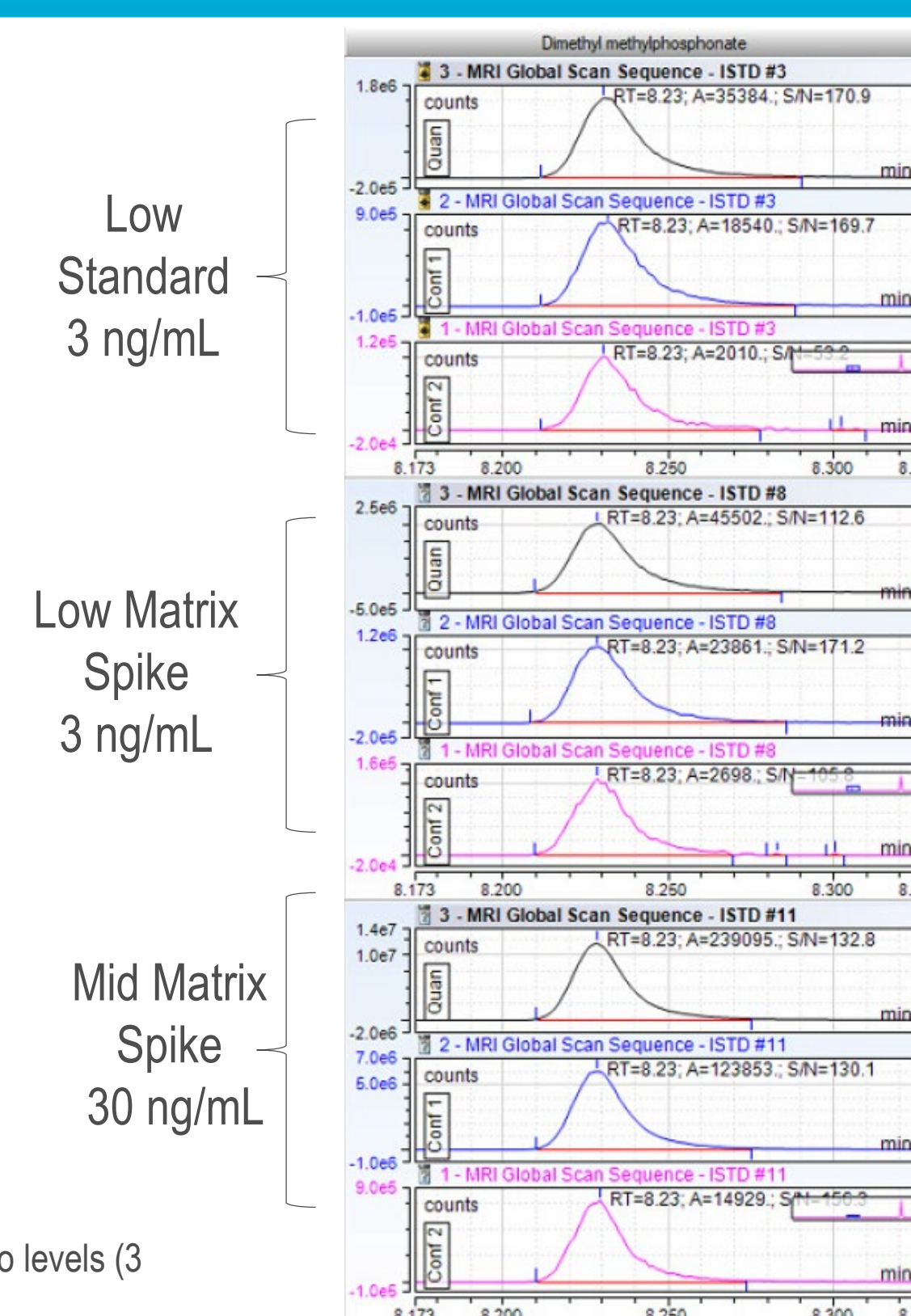
The purpose of the initial evaluation was to find a GC-HRMS instrument to replace the aging magnetic sector GC-HRMS (AutoSpec).

Prior to purchasing the Orbitrap, analytical standards and matrix sample extracts (18 chemicals) were sent to an Orbitrap specialist to determine sensitivity, linearity, precision, and accuracy of the Orbitrap Exploris GC-HRMS. The Thermo Orbitrap specialist developed a method and SIM scan parameters, analyzed the standards and sample extracts, and provided a report.

Initial evaluation of the Orbitrap provided the necessary data showing the Orbitrap to be a suitable GC-HRMS instrument for MRIGlobal projects.

The Orbitrap Exploris 30K GC-HRMS was installed in October 2021.

Figure 4 (right). SIM data of Dimethyl methylphosphonate standards run by Thermo at two levels (3 ng/mL and 30 ng/mL) along with a mid matrix spike extract.



Traditional Chemical Agents - SIM Data

The Orbitrap's SIM mode increases sensitivity by filtering out extraneous masses in the quadrupole. The masses of interest are allowed to collect in the C-Trap before being sent to the mass analyzer. The time allowed to collect, the range of masses let through the filter, and number of ions sent to the detector are scan parameters that can be independently adjusted to optimize sensitivity.

All analytes have excellent linearity and sensitivity at low level concentrations.

Table 1. Traditional Chemical Agent's Low Standard Concentration and Linearity Values

Analyte	Orbitrap Approx. Low Std. ng/mL	R ² Value Calibration Range 20X
GB	1.0	0.9999
GD	2.5	0.9998
HN-2	0.60	0.9999
HN-1	0.80	0.9998
HN-3	0.80	0.9999
HD	3.0	0.9996
GA	10	0.9996
GF	9.0	0.9996
VX	11	0.9982
RVX	3.2	0.9977

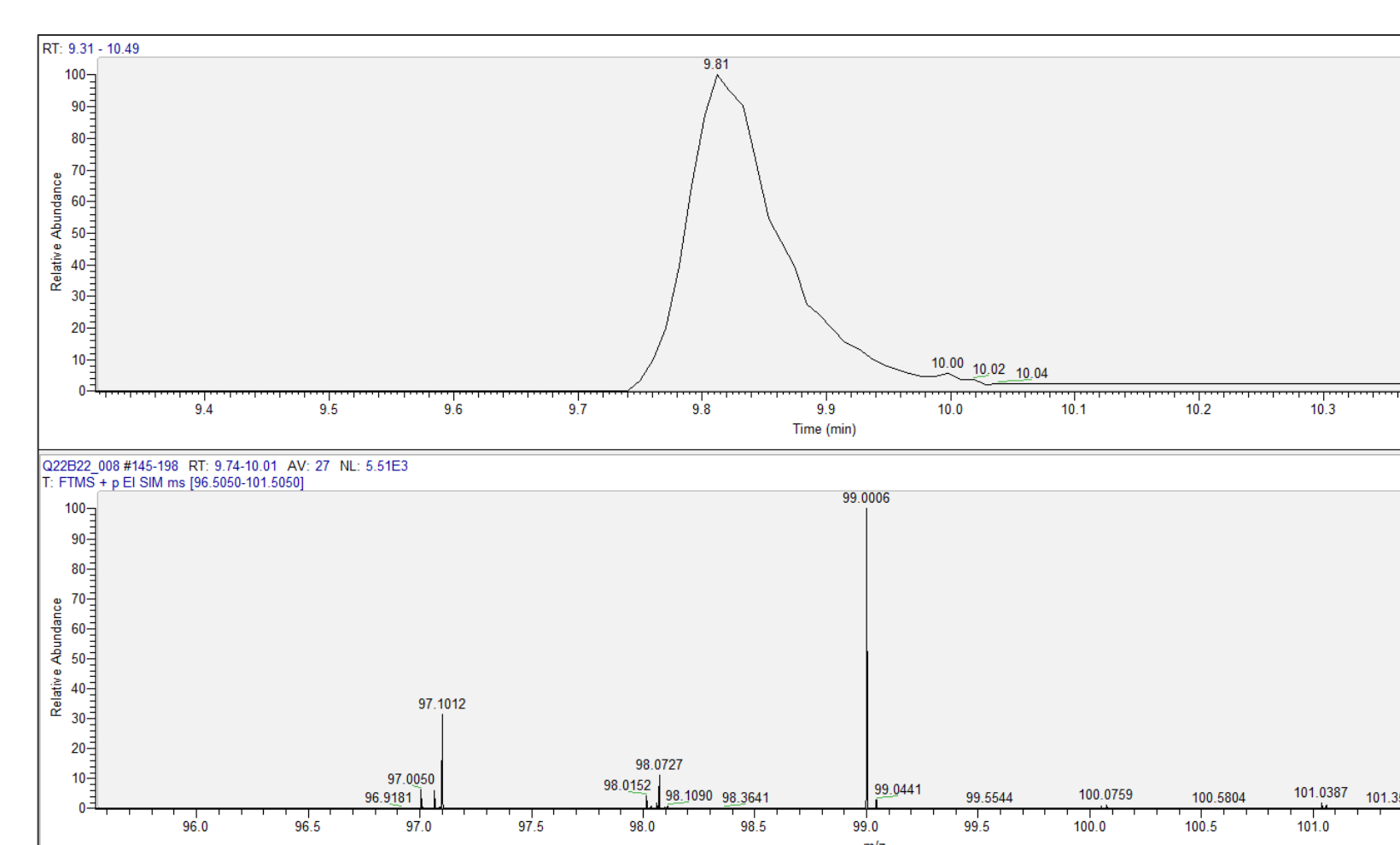


Figure 5. SIM data of 1.0 ng/mL GB standard showing m/z range allowed to detector, and 99.0005 m/z extracted

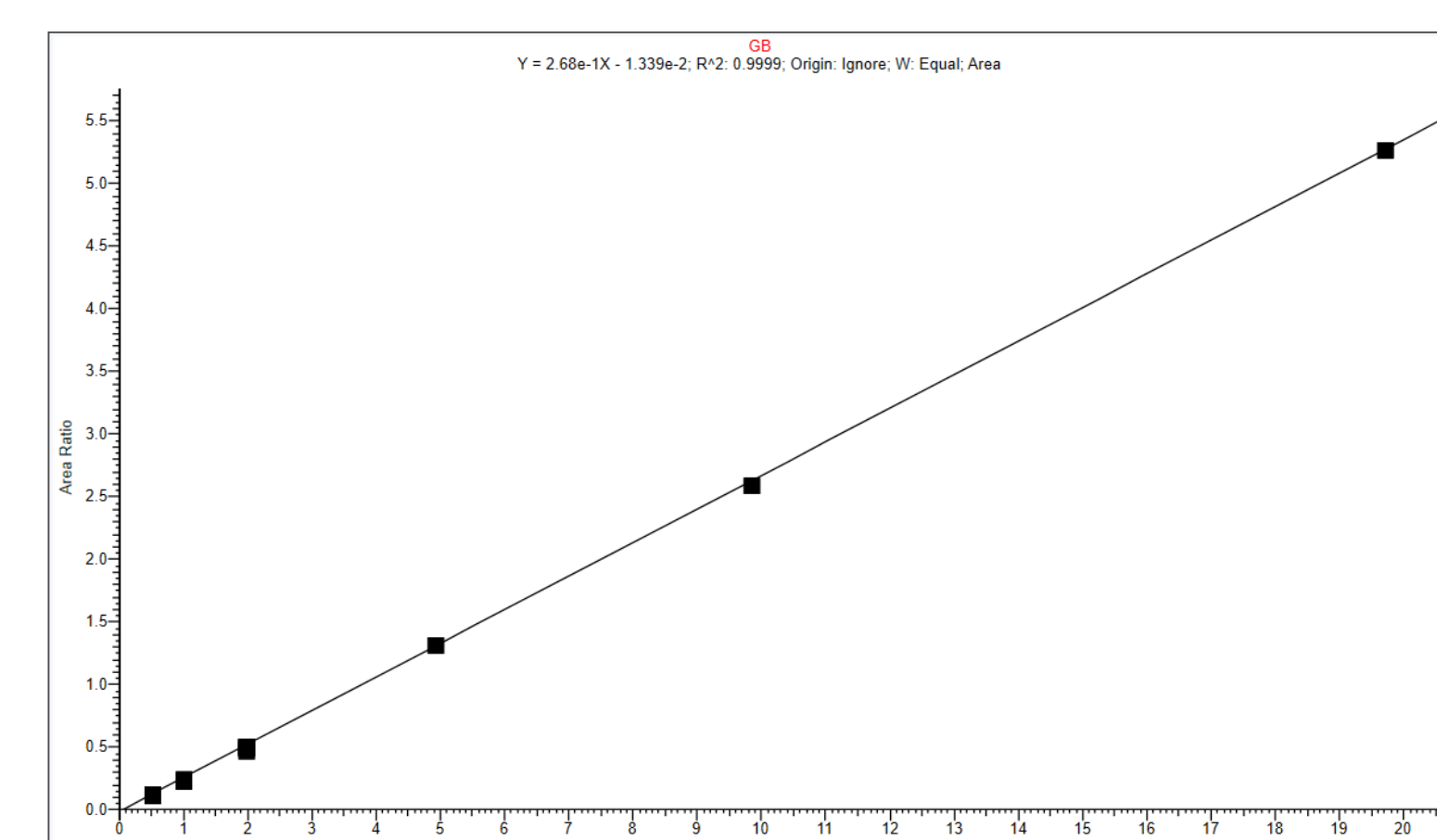


Figure 6. Calibration curve generated in TraceFinder of GB (99.0005 m/z).

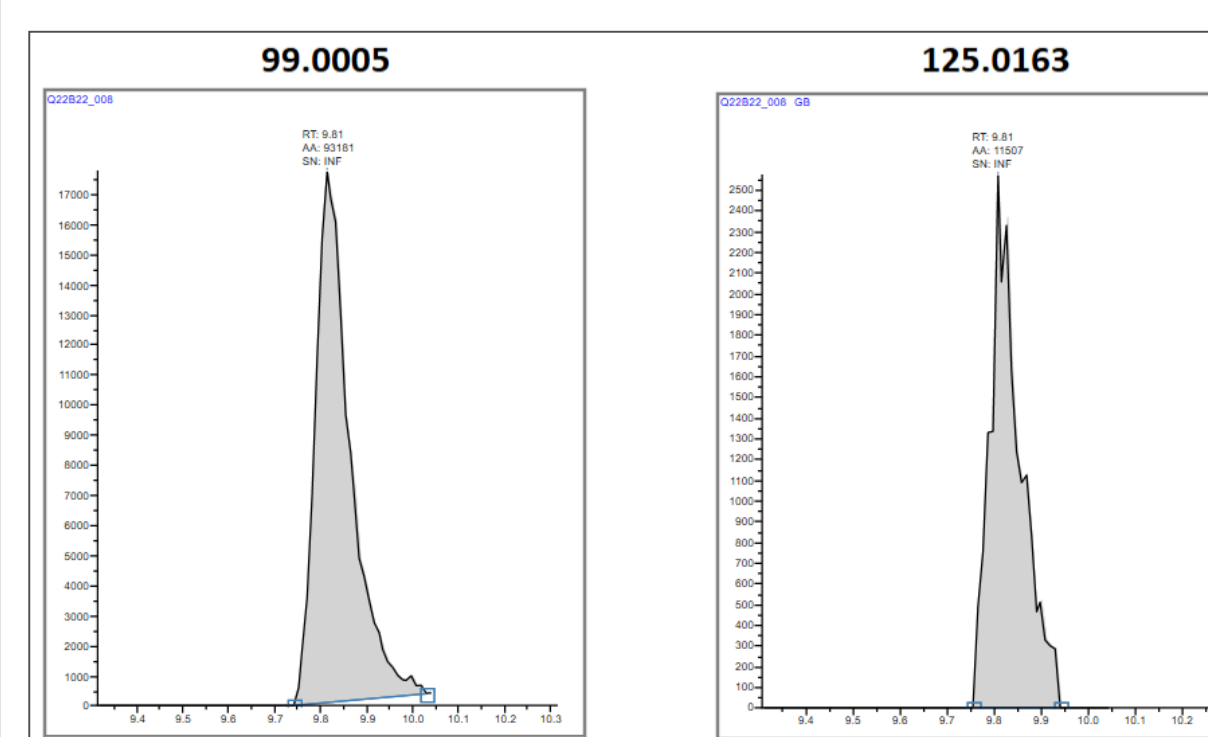
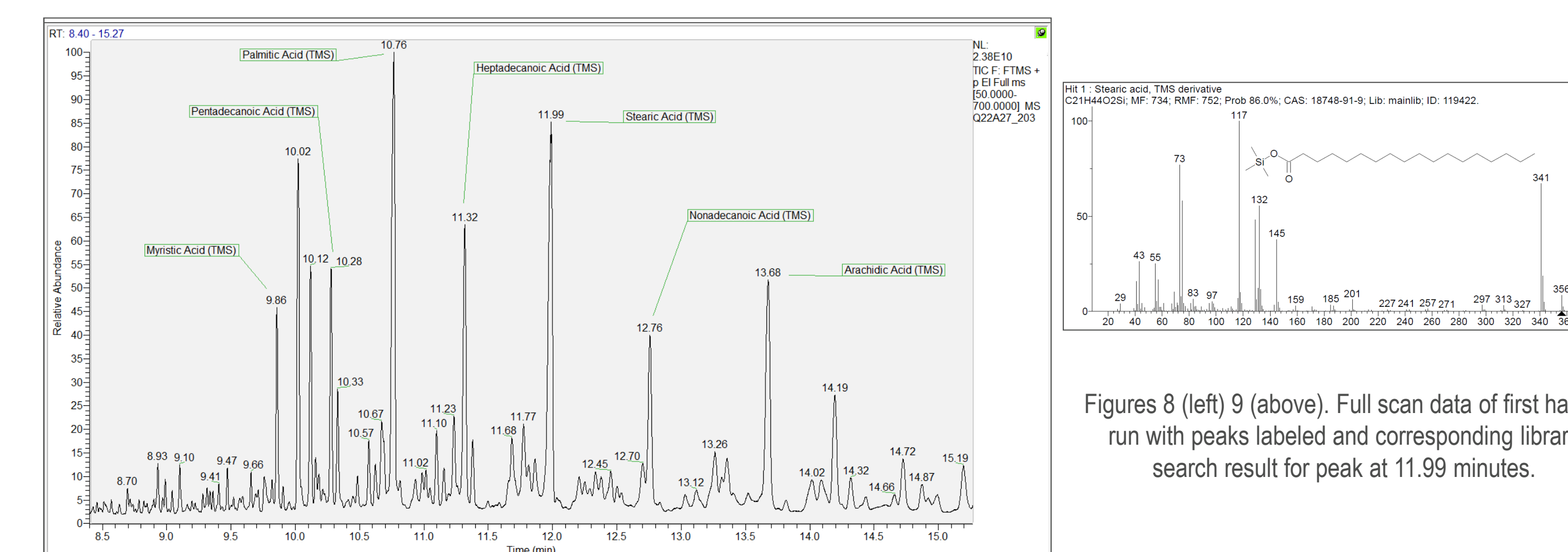


Figure 7 (above). Extracted ion chromatograms for the quantitation (99.0005 m/z) and confirming (125.0163 m/z) ions of GB at 1.0 ng/mL.

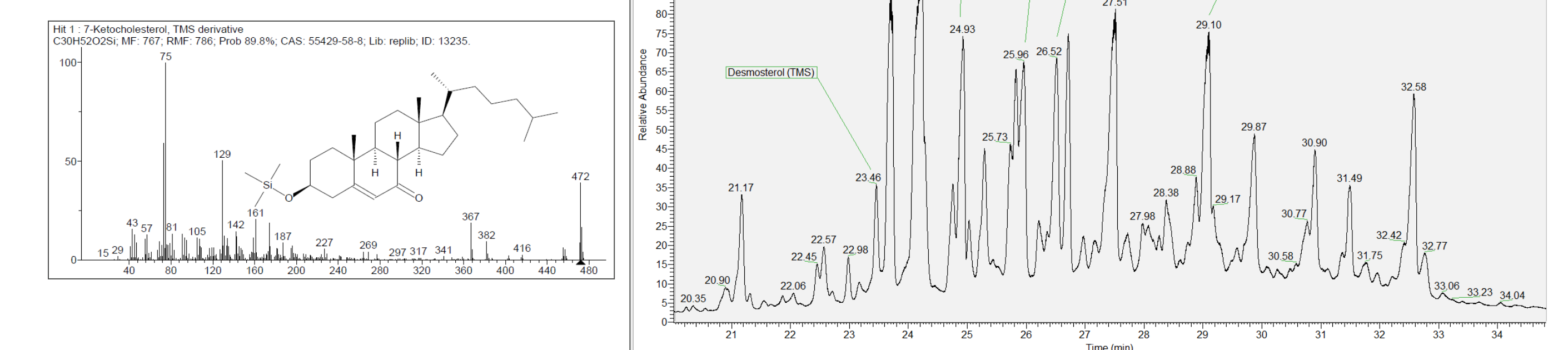
Full scan / Unknown Identification

Full scan screening of unknowns can be performed with data compared against NIST or Wiley libraries. The software contains a deconvolution plugin which allows coeluting peaks to be separated based on minute retention time differences. Users can then create a searchable in-house high-res database. A comparison of the Orbitrap was performed against a low-resolution GC/MS. Notably, the Orbitrap had better sensitivity and higher confidence matches compared to the low-resolution GC/MS. Ultimately, the Orbitrap data was reported.



Figures 8 (left) 9 (above). Full scan data of first half of run with peaks labeled and corresponding library search result for peak at 11.99 minutes.

Figures 10 (right) and 11 (below). Full scan data of later end of run with peaks labeled and corresponding library search result for peak at 29.10 minutes.



Conclusions

The Orbitrap Exploris 30K is an effective and sensitive GC-HRMS instrument which can yield meaningful data in full scan or SIM modes. The Orbitrap Exploris 30K has MS/MS capabilities that have not yet been explored, which could provide even more sensitive results.

The Orbitrap Exploris 30K's ease of use and modular design allows for quick acquisition, adaptability, and customization based on the need and purpose of the work. Data processing in TraceFinder is streamlined and the report editor allows for customized deliverables.

Contact Mary Duncan or Cristi Gillom with questions concerning applications to project needs.

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